



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 01:12 pm GMT

PDB ID : 1JG0
Title : Crystal structure of Escherichia coli thymidylate synthase complexed with 2'-deoxyuridine-5'-monophosphate and N,O-didansyl-L-tyrosine
Authors : Fritz, T.A.; Tondi, D.; Finer-Moore, J.S.; Costi, M.P.; Stroud, R.M.
Deposited on : 2001-06-22
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

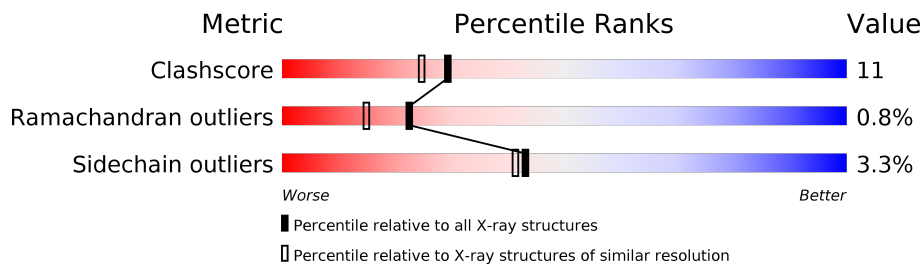
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	
1	B	264	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4846 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

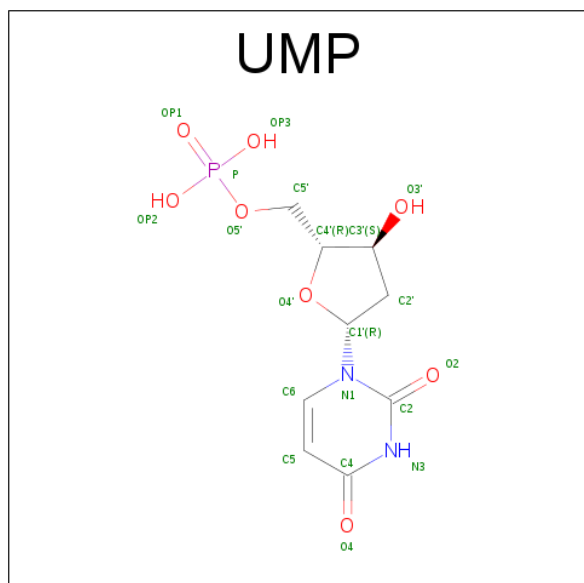
- Molecule 1 is a protein called thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	3	0
			2159	1378	372	396	13			
1	B	263	Total	C	N	O	S	0	3	0
			2159	1378	372	396	13			

There are 6 discrepancies between the modelled and reference sequences:

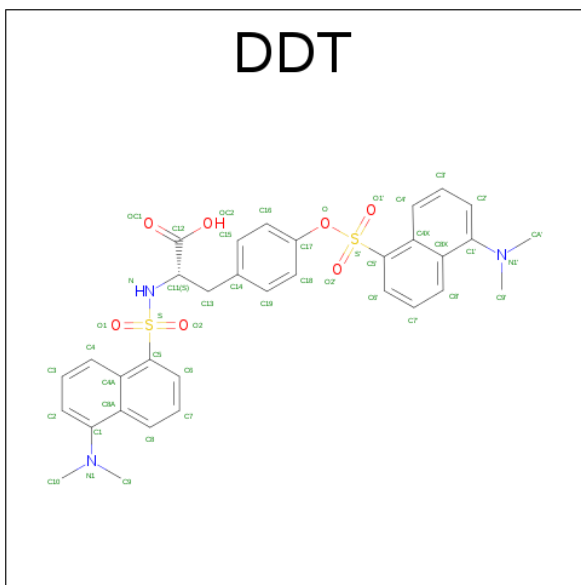
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	MODIFIED RESIDUE	UNP P0A884
A	21	ALA	ARG	CONFLICT	UNP P0A884
A	107	ALA	ARG	CONFLICT	UNP P0A884
B	1	CXM	MET	MODIFIED RESIDUE	UNP P0A884
B	21	ALA	ARG	CONFLICT	UNP P0A884
B	107	ALA	ARG	CONFLICT	UNP P0A884

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 20	C 9	N 2	O 8	P 1	0	0
2	B	1	Total 20	C 9	N 2	O 8	P 1	0	0

- Molecule 3 is N,O-DIDANSYL-L-TYROSINE (three-letter code: DDT) (formula: $C_{33}H_{33}N_3O_7S_2$).

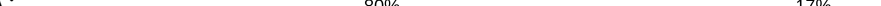



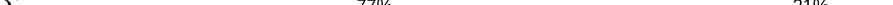

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 45	C 33	N 3	O 7	S 2	0	0
3	B	1	Total 45	C 33	N 3	O 7	S 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	219	Total O 219 219	0	0
4	B	179	Total O 179 179	0	0

Note EDS was not executed.

- Chain A:  80% 17%
- 
- | Position | Completion Status |
|----------|-------------------|
| K1 | 80% |
| K2 | 80% |
| E6 | 80% |
| K18 | 80% |
| G25 | 80% |
| S28 | 80% |
| H32 | 80% |
| N37 | 80% |
| L38 | 80% |
| Q39 | 80% |
| L44 | 80% |
| L52 | 80% |
| L59 | 80% |
| K83 | 80% |
| A84 | 80% |
| G88 | 80% |
| D89 | 80% |
| Y94 | 80% |
| Q97 | 80% |
| W101 | 80% |
| P102 | 80% |
| T103 | 80% |
| P104 | 80% |
| D105 | 80% |
| G106 | 80% |
| A107 | 80% |
| L116 | 80% |
| W133 | 80% |
| M134 | 80% |
| L138 | 80% |
| M141 | 80% |
| L142 | 80% |
| L143 | 80% |
| C146 | 80% |
| H147 | 80% |
| A148 | 80% |
| F149 | 80% |
| L153 | 80% |
| C167 | 80% |
| C168 | 17% |
| L174 | 17% |
| N177 | 17% |
| L183 | 17% |
| Q190 | 17% |
| D193 | 17% |
| H207 | 17% |
| L208 | 17% |
| Q215 | 17% |
| L227 | 17% |
| I231 | 17% |
| I232 | 17% |
| K235 | 17% |
| P236 | 17% |
| I239 | 17% |
| Y242 | 17% |
| E248 | 17% |
| I249 | 17% |
| A263 | 17% |
| ILE | 17% |

- Chain B:  77% 21%
- 
- | Position | Amino Acid | Frequency (approx.) |
|----------|------------|---------------------|
| 1 | W1 | 0.25 |
| 2 | K10 | 0.25 |
| 3 | N19 | 0.25 |
| 4 | D20 | 0.25 |
| 5 | A21 | 0.25 |
| 6 | T22 | 0.25 |
| 7 | G23 | 0.25 |
| 8 | T24 | 0.25 |
| 9 | H32 | 0.25 |
| 10 | Q33 | 0.25 |
| 11 | L38 | 0.25 |
| 12 | H51 | 0.25 |
| 13 | H57 | 0.25 |
| 14 | Y71 | 0.25 |
| 15 | N76 | 0.25 |
| 16 | I79 | 0.25 |
| 17 | Y94 | 0.25 |
| 18 | W101 | 0.25 |
| 19 | P102 | 0.25 |
| 20 | T103 | 0.25 |
| 21 | P104 | 0.25 |
| 22 | D105 | 0.25 |
| 23 | G106 | 0.25 |
| 24 | A107 | 0.25 |
| 25 | I112 | 0.25 |
| 26 | V115 | 0.25 |
| 27 | L116 | 0.25 |
| 28 | H117 | 0.25 |
| 29 | Q118 | 0.25 |
| 30 | D124 | 0.25 |
| 31 | R127 | 0.25 |
| 32 | I128 | 0.25 |
| 33 | M134 | 0.25 |
| 34 | V135 | 0.25 |
| 35 | L143 | 0.25 |
| 36 | A144 | 0.25 |
| 37 | P145 | 0.25 |
| 38 | C146 | 0.25 |
| 39 | H147 | 0.25 |
| 40 | A148 | 0.25 |
| 41 | F149 | 0.25 |
| 42 | I152 | 0.25 |
| 43 | S167 | 0.25 |
| 44 | L172 | 0.25 |
| 45 | M177 | 0.25 |
| 46 | Y181 | 0.25 |
| 47 | A182 | 0.25 |
| 48 | L183 | 0.25 |
| 49 | D193 | 0.25 |
| 50 | W201 | 0.25 |
| 51 | Y209 | 0.25 |
| 52 | S210 | 0.25 |
| 53 | N211 | 0.25 |
| 54 | H212 | 0.25 |
| 55 | M213 | 0.25 |
| 56 | D214 | 0.25 |
| 57 | Q215 | 0.25 |
| 58 | R222 | 0.25 |
| 59 | L230 | 0.25 |
| 60 | I231 | 0.25 |
| 61 | F244 | 0.25 |
| 62 | E245 | 0.25 |
| 63 | T246 | 0.25 |
| 64 | D247 | 0.25 |
| 65 | E248 | 0.25 |
| 66 | I249 | 0.25 |
| 67 | H255 | 0.25 |
| 68 | P256 | 0.25 |
| 69 | P261 | 0.25 |
| 70 | V262 | 0.25 |
| 71 | A263 | 0.25 |
| 72 | I1E | 0.25 |

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.80Å 87.06Å 127.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.42 – 2.00	Depositor
% Data completeness (in resolution range)	99.6 (27.42-2.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4846	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DDT, CXM, UMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/2209	0.71	1/3002 (0.0%)
1	B	0.43	0/2209	0.72	3/3002 (0.1%)
All	All	0.43	0/4418	0.72	4/6004 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ASN	N-CA-C	-6.32	93.94	111.00
1	A	208	LEU	CA-CB-CG	5.21	127.27	115.30
1	B	20	ASP	N-CA-C	5.18	125.00	111.00
1	B	149	PHE	N-CA-CB	-5.12	101.39	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2159	0	2076	44	0
1	B	2159	0	2076	47	0
2	A	20	0	11	0	0
2	B	20	0	11	0	0
3	A	45	0	32	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	45	0	32	2	0
4	A	219	0	0	5	0
4	B	179	0	0	8	0
All	All	4846	0	4238	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 94 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:GLN:HE21	1:B:215:GLN:H	1.10	0.97
1:B:215:GLN:NE2	1:B:215:GLN:H	1.66	0.92
1:A:215:GLN:HE21	1:A:215:GLN:H	1.15	0.90
1:A:215:GLN:NE2	1:A:215:GLN:H	1.76	0.83
1:A:52:LEU:HD12	1:A:249:ILE:HD11	1.66	0.77

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	264/264 (100%)	250 (95%)	12 (4%)	2 (1%)	22	15
1	B	264/264 (100%)	247 (94%)	15 (6%)	2 (1%)	22	15
All	All	528/528 (100%)	497 (94%)	27 (5%)	4 (1%)	22	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	ASP

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Mol	Chain	Res	Type
1	A	94	TYR
1	B	94	TYR
1	B	104	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/230 (101%)	224 (97%)	8 (3%)	42	40
1	B	232/230 (101%)	225 (97%)	7 (3%)	46	46
All	All	464/460 (101%)	449 (97%)	15 (3%)	43	42

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	227	LEU
1	B	172	LEU
1	A	149	PHE
1	B	143	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	B	19	ASN
1	B	151	GLN
1	A	217	HIS
1	B	32	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CXM	A	1	1	7,10,11	1.05	1 (14%)	5,11,13	1.04	0
1	CXM	B	1	1	7,10,11	1.18	2 (28%)	5,11,13	1.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	A	1	1	-	0/6/10/12	0/0/0/0
1	CXM	B	1	1	-	0/6/10/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	CXM	CA-N	2.02	1.49	1.46
1	B	1	CXM	CA-C	2.15	1.53	1.50
1	A	1	CXM	CA-N	2.46	1.49	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	UMP	A	303	-	17,21,21	3.32	4 (23%)	23,31,31	2.32	4 (17%)
3	DDT	A	304	-	46,49,49	1.95	9 (19%)	65,73,73	1.44	10 (15%)
2	UMP	B	305	-	17,21,21	3.53	4 (23%)	23,31,31	2.62	4 (17%)
3	DDT	B	306	-	46,49,49	2.03	7 (15%)	65,73,73	1.45	10 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMP	A	303	-	-	0/6/22/22	0/2/2/2
3	DDT	A	304	-	-	0/34/38/38	0/5/5/5
2	UMP	B	305	-	-	0/6/22/22	0/2/2/2
3	DDT	B	306	-	-	0/34/38/38	0/5/5/5

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	306	DDT	O-C17	-2.93	1.38	1.42
3	A	304	DDT	C7-C6	2.05	1.42	1.38
3	A	304	DDT	C7'-C6'	2.07	1.42	1.38
3	A	304	DDT	C3-C2	2.09	1.42	1.38
3	B	306	DDT	C9'-N1'	2.35	1.51	1.45

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	306	DDT	C2-C1-N1	-3.71	115.99	121.70
2	B	305	UMP	C2'-C1'-N1	-3.12	106.87	114.23

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	304	DDT	C2'-C1'-N1'	-3.03	117.03	121.70
3	B	306	DDT	C4-C4A-C5	-2.79	120.05	123.63
3	B	306	DDT	C4A-C5-S	-2.63	118.33	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	DDT	3	0
3	B	306	DDT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.